

Statement of Research for Quanlin Zhou

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During my tenure at LBNL from March 2001 to the present, I have been working on (1) geologic carbon sequestration projects for mitigating global climate change, (2) the Yucca Mountain project for characterizing the geologic repository site for nuclear waste disposal, and (3) site-specific contamination remediation and assessment projects. My research at LBNL focuses on the following four areas.

1. Analytical and Numerical Modeling of Geologic Carbon Sequestration (GCS) [J1–J6, J8–J10]

In order to make GCS an effective measure for climate change mitigation, we face three grand challenges: (1) subsurface storage capacity is constrained by pressure buildup and its adverse effects (e.g., caprock integrity damage, induced seismicity, and fault reactivation); (2) the effects of subsurface heterogeneity on CO₂ migration, long-term trapping, and storage efficiency need to be better quantified; and (3) monitoring and joint inversion methods for early warning and detection of CO₂ leakage need development. In the past five years, I focused my research on (1), via analytical and numerical modeling.

My research in the area of high-performance, numerical modeling of CO₂-brine flow and single-phase brine flow focuses on (1) understanding pressure buildup and brine migration induced by GCS in closed, semi-closed, and open sedimentary basins with simplified systems [J9, J10], (2) evaluating the dynamic storage capacity and impact of GCS on groundwater resources in the Illinois Basin and the southern San Joaquin Basin, as examples, to understand the full-scale deployment and pressure-constrained dynamic storage capacity under operation [J3, J5, J6], and (3) assessing brine leakage through abandoned wells, including nonisothermal effects [J2]. My research shows the limiting effect of pressure buildup on dynamic storage capacity to avoid adverse geomechanical and environmental effects, although the constraint is moderated by pressure propagation in the storage formation and pressure bleed-off into overlying/underlying formations. The secondary-seal effect was manifested by retarding upward CO₂ migration through multiple secondary (more permeable) seals, coupled with lateral CO₂ viscous fingering through high-permeability layers [J5, J6].

My research also includes development and application of new analytical solutions to single-phase brine flow: (1) a solution developed for pressure perturbations and leakage in a laterally bounded aquifer-aquitard system, complementing the solutions for infinite systems developed by Theis, Hantush, Neuman, and Moench [J4, J8], and (2) a solution developed for pressure perturbations and leakage through aquitards and leaky abandoned wells in a multilayered system, generalizing well hydraulics to a system of any number of aquifers, alternative semi-pervious aquitards, injection wells, and leaky wells [J1]. The super-computational efficiency of these solutions facilitates analyzing the sensitivity of pressure buildup and brine-flow rate to hydrogeologic properties of storage formation, seals, and leaky structures, developing pressure management schemes using inverse modeling, and providing insights into leakage detection using pressure data.

2. Field-Scale Diffusive Transport in Fractured and Porous Media [J11, J13–J16]

Diffusive transport has been demonstrated to be one of the key transport phenomena in fractured rock, through mathematical modeling, laboratory experiments, and field tracer tests. However, its behavior in the field is more complicated because of the interplay of advection and dispersion in fracture networks with diffusion in the rock matrix of naturally heterogeneous systems. Along with other colleagues, I have proposed and systematically demonstrated that the field-scale, effective matrix diffusion coefficient for heterogeneous fractured rock might be dependent on the observation scale, following the findings of scale-dependent hydraulic conductivity and macrodispersivity. This conclusion was based on our studies of a critical literature review, numerical experiments, and tracer-test analyses: (1) a comprehensive critical review was conducted for all field-scale tracer tests in the literature, showing that the field-scale, effective matrix diffusion coefficient is scale-dependent [J13]; (2) numerical experimental results indicate scale-dependent behavior, with a slope dependent on the local matrix diffusion coefficient, aperture ratios between different levels of fractures, and the scaling feature for the network of multiscale (length, aperture) fractures [J14]; (3) numerical experiments indicate that the spatial variability of the local-scale matrix diffusion coefficient along single or multiple parallel flow paths does not contribute to the observed scale-dependent

behavior [J15]; (4) modeling analysis of a long-term field-scale tracer test shows spatial variability of the local-scale matrix diffusion coefficient within the rock matrix in the direction perpendicular to the fracture-matrix wall [J16]. This scale-dependent behavior stems from the heterogeneous network of multiscale fractures, rather than the spatial variability in the local-scale matrix diffusion coefficient. This observation may have strong implications with respect to enhanced solute or radionuclide retardation in fractured rock.

In contrast to our observations regarding fractured rock, Haggerty et al. [2004] found that the mass-transfer rate coefficient in porous media decreases with experimental duration or residence time, using analyses of 316 transport experiments. Following the analyses of numerous experiments using the first-order mass-transfer model, we analyzed the MADE-2 tracer test and concluded that the field-scale mass-transfer rate coefficient decreases over tracer residence time. However, we challenged Haggerty et al.'s [2004] conclusions, finding that this scale-dependent behavior is mainly an artifact of numerical model approximations, rather than the real physical process of multirate diffusion [J11].

3. Flow and Transport in Heterogeneous Fractured/Porous Media [J7, J12, J17– J20]

I have focused my research on a broader area of flow and transport in heterogeneous, saturated/unsaturated fractured/porous media. This research has included (1) characterization of multiscale heterogeneity of hydrogeologic properties in the fractured unsaturated zone at Yucca Mountain, and prediction of unsaturated flow and solute transport in heterogeneous fractured rock [J20]; (2) analysis of a mesoscale infiltration and seepage test and correlation between infiltration/seepage rates and mapped fractured patterns through modeling and field observations [J17]; (3) development of a density-dependent flow simulator and application of it to saltwater upconing and decay beneath a well pumping [J18]; (4) calibration of saturated groundwater flow at a DNAPL-contaminated site (in support of on-site remediation) [J19]; and (5) discovery of field evidence for significant *in situ* biodegradation of N-Nitrosodimethylamine (NDMA), through field monitoring and numerical modeling of a large-scale groundwater system receiving recycled water as incidental and active recharge [J7].

4. Subsurface Heterogeneity Tomography and Early Warning and Detection of CO₂ Leakage

With five ongoing projects and support from four postdocs, I am developing two new research interests. My first new research interest is the investigation of CO₂ migration, long-term trapping, and storage efficiency in hierarchical, multiscale heterogeneous sedimentary rock, and the development of the methodology of subsurface heterogeneity tomography (SHT) (Challenge 2). I developed conceptual models for a number of key transport processes in heterogeneous formations: (1) viscous fingering of free-phase CO₂ along high-permeability (or high-K) fast-flow pathways; (2) dynamic intrusion of CO₂ from high-K zones into relatively low-K zones by capillarity and buoyancy; (3) diffusive transport of dissolved CO₂ into low-K zones across large interface areas created by CO₂ fingers; and (4) density-driven convective mass transfer into CO₂-free regions confined by shale layers. These CO₂ migration and trapping processes are investigated at core scale (centimeters, working with a partner in China), at laboratory scale (1–5 m), at field pilot scale at the Frio site (~100 m), and at large storage scale at Kevin Dome, Montana (kilometers). In addition, the SHT methodology will be developed using hydraulic-thermal-tracer-CO₂ storage tests in the field, borehole logs, and other raw hydrogeologic data. SHT will be tested and applied to the Frio Pilot Test, a small-scale CO₂ storage experiment that offers a wealth of diverse monitoring data for hydraulic, thermal, tracer, and CO₂ injection tests.

My second new research interest involves early warning and detection of CO₂ leakage through seal imperfections (e.g., fractures, abandoned wells, and fault zones) by real-time monitoring of fast-propagating pressure and ground-surface uplift at a large scale and of slow-migrating CO₂ plume at the plume scale, and by deterministic and stochastic joint inversion (Challenge 3). The key to early leakage detection is to detect pressure-driven brine leakage through leakage pathways as early as possible, to predict the relatively slow CO₂ plume migration in the storage reservoir for CO₂ leakage, and to guide deployment of monitoring for improving data and detection, with the ultimate goal of mitigating leakage risks. This new technology is under development—it will be tested and applied to the CO₂ injection and storage at the Ketzin, Germany site, and at the In Salah, Algeria site, with sufficient data and potential fault leakage of CO₂/brine.